

β -SeO₂ Structure: A2B_oP12_26_abc_ab-002

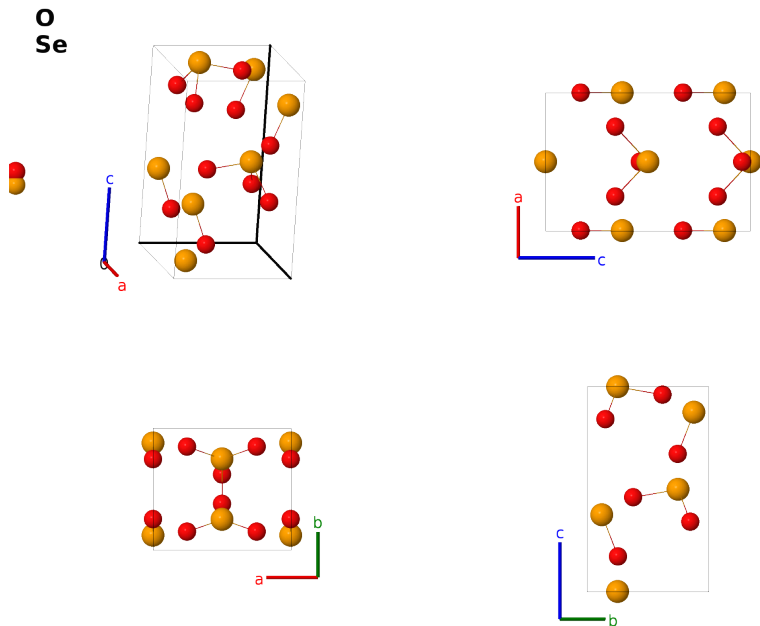
This structure previously used the label(s) **A2B_oP12_26_abc_ab.Se02**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/2MYY>

https://aflow.org/prototype-encyclopedia/A2B_oP12_26_abc_ab-002



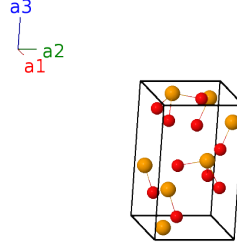
Prototype	O ₂ Se
AFLOW prototype label	A2B_oP12_26_abc_ab-002
ICSD	99464
CCDC	1658690
Pearson symbol	oP12
Space group number	26
Space group symbol	<i>Pmc</i> 2 ₁
AFLOW prototype command	<code>aflow --proto=A2B_oP12_26_abc_ab-002</code> <code>--params=a, b/a, c/a, y₁, z₁, y₂, z₂, y₃, z₃, y₄, z₄, x₅, y₅, z₅</code>

- SeO₂ has been observed in three phases (Orosel, 2004):
 - Downeyite, α -SeO₂, *Strukturbericht C47*, the ground state,

- β -SeO₂ (this structure), and
- γ -SeO₂.
- The later two phases form at high pressures (up to 15GPa and 820°C) but upon quenching and slowly reducing the pressure they remain metastable under ambient conditions.
- Data for β -SeO₂ was taken at 200K using powder diffraction data.
- Space group $Pmc2_1$ #26 allows an arbitrary choice for the origin of the z -axis. Here we follow (Orosel, 2004) and set $z_4 = 0$ for the Se II (2b) site.
- β -SeO₂ has the same AFLOW label as 70 GPa H₂S, A2B.oP12_26_abc.ab. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_2$	$= -y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_3$	$= y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2a)	Se I
$\mathbf{B}_4$	$= -y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Se I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2b)	Se II
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Se II
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{11}$	$= x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{12}$	$= -x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	O III

References

- [1] D. Orosel, O. Leynaud, P. Balog, and M. Jansen, *Pressure–temperature phase diagram of SeO₂. Characterization of new phases*, J. Solid State Chem. **177**, 1631–1638 (2004), doi:10.1016/j.jssc.2003.12.028.

Found in

- [1] P. Villars and K. Cenzual, *Pearson’s Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043